Study of Electronic properties of III-V semiconductors and semiconductor-superlattices

A thesis submitted in the partial fulfilment of the requirement for the Degree of

Integrated MSc

IN

PHYSICS

By

Banoj Kumar Nayak

Roll No – 409PH5006

Under guidance of

Dr. Biplab Ganguli

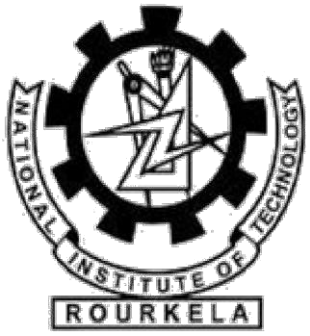
Dept. of Physics and Astronomy

National Institute of Technology, Rourkela

Declaration

I do hereby declare that the research work incorporated in the thesis entitled ”Study of Electronic properties of III-V semiconductors and semiconductor-superlattices” is an original research work carried out by us in the Department of Physics, NIT Rourkela, under the supervision and guidance of Dr.Biplab Ganguli.

Date:09/05/2014 Banoj Kumar Nayak



DEPARTMENT OF PHYSICS AND ASTRONOMY

NIT ROURKELA

CERTIFICATE

This is to certify that the thesis entitled "Study of Electronic properties of III-V semiconductors and semiconductor-superlattices" submitted by Mr Banoj Kumar Nayak, Integrated MSc student of Department of Physics and Astronomy, National Institute of Technology, Rourkela in partial fulfilment for the requirement for the award of degree of Master of Science degree in Physics has been carried out by him under my supervision and guidance. The results incorporated in the thesis have been reproduced by TB-LMTO code.

Prof. Biplab Ganguli
Dept. of Physics and Astronomy
National Institute Technology
Rourkela-769008

ACKNOWLEDGEMENT

I heartily express my deepest sense of gratitude to my supervisor Dr. Biplab Ganguli, NIT Rourkela for his suggestion and guidance .His great interest, encouragement and guidance had made my work fruitful.

I express my special thanks to the research scholars, Computational Physics Lab for their valuable suggestions and guidance throughout my dissertion work.

Date: 09/05/2014 Banoj Kumar Nayak

ABSTRACT

We have studied different methods for calculating band structures of solids and their density of states which can predict the electronic properties of solids accurately. Especially, computational methods like tight binding approximation and pseudo potential method have been studied and applied to find the band structures and density of states of semiconductors and its superlattices. The project work is divided into two parts. In first part, pseudo potential method has been used to solve computationally by MATLAB, the energy Eigen values of III-V semiconductors like GaAs and AlAs and IV semiconductor i.e. Ge and get a graphical representation of their band structures. In second part, TB-LMTO program which uses tight binding method has been applied to find the band structures and density of states of GaAs and AlAs semiconductors and their superlattices (GaAs/AlAs). A comparison of conducting behaviour of these materials is made finally.

TABLE OF CONTENTS

Introduction

Semiconductor:

Semiconductors have band gap in between that of an insulator and conductor. Normally, it varies from .5ev to 5ev. So, their conductivity are less than conductor and more than insulator. The bands are not completely filled in semiconductors. So electrons can contribute to transport properties in semiconductors. Normally, at low temperature, they behave as insulator. But, at relatively high temperature, the charge carriers get enough thermal energy to overcome the energy barrier of forbidden band gap and jump from valence band to conduction band.

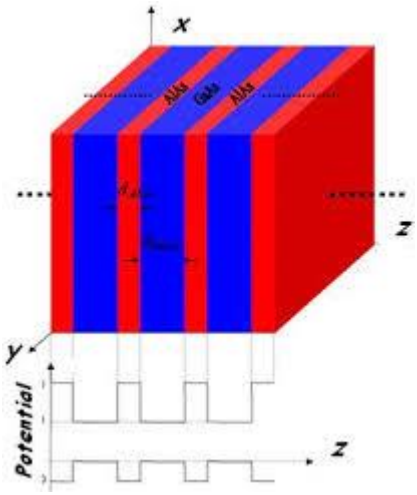
GaAs and AlAs semiconductors have structures like that of zinc-blende. Ge has structure of diamond type. Both diamond and zinc-blende structure consists of two fcc lattices interpenetrated with each other. One fcc primitive cell is shifted along the body diagonal of one-fourth length of another lattice. In diamond structure, the atoms in both the fcc lattices are same whereas in zinc-blende structures two different types of atoms are present at two different lattices.

Semiconductor superlattices:

Superlattices are periodic repetition of two alternating layers of different materials. Basically, the periodicity or repetition unit is larger than the length of the lattice constant. The growth of superlattices is made by artificial techniques. Crystals of Semiconductor superlattices are alternate layers of two different type of semiconductors. The lattice constants of both the semiconductors are taken to be same. But the band gaps are different for them. Variation in band gaps is done in two ways. In first way, it is done by taking same semiconductor with adding donor or acceptor atoms in alternate layers. So, the electrons are localized in one region and holes are localized in other region. However, in this method there is chance of diffusion of holes and electrons overcoming the energy barrier of band gaps of two layers. In second way, it is done by taking two different semiconductors with different compositions. This method is widely used since there will be no diffusion and potential barrier will be maintained between two layers. The examples of such semiconductor superlattices are $(GaAs)_n/(AlAs)_m$, where n layers of GaAs and m layers of AlAs are present in one unit cell of superlattice.

Again, the superlattices is of two types w.r.t. confinement of holes and electrons. In type-1 superlattices, the conduction band edge of one material is higher than that of others, but valence band edge is lower than the other. So, both hole and electrons are confined in the same region i.e. the barriers and wells are same for both of them. In type-2 superlattice, both valence band edges and conduction band edges are more than the other material. So, barrier and wells are different for electrons and holes. So, they are confined in different regions. $(GaAs)_n/(AlAs)_m$ is a type-1 superlattice.

The layers of GaAs and AlAs are repeated as shown in figure in $(GaAs)_1/(AlAs)_1$.



Computational methods:

There are various methods to calculate the band structures. They are tight binding method, green function method, KKR method, pseudo potential method etc.

Pseudo potential method:

Pseudo potential method is an effective method and advantageous since it gives the same accurate result with less number of time. In this method, the core electrons are frozen out with the nucleus. Only valence electrons are considered for calculating the band structures. In this method, a pseudo potential is used instead of the original ionic potential in the Hamiltonian. The original ionic potential produces the real crystal wave functions for valence electrons which are rapidly oscillatory in the core region of nucleus and smoothly varying like plane waves in interstitial region. This wave function is a linear combination of large number of plane waves. However, the pseudo potential is defined like the way such that it is a smoothly varying function in the core region also. So, the pseudo wave function produced by this potential is a smoothly varying and can be represented as a linear combination of less number of plane waves. Although the pseudo wave function is different from real wave function, the energy Eigen values remains the same as real case.

The real crystal wave function is represented as a combination of pseudo wave function and core states such that it is orthogonal to core states.

$$\psi_\kappa = \phi_k - \sum <\Phi_{k,t} / \phi_k > \Phi_{k,t}$$

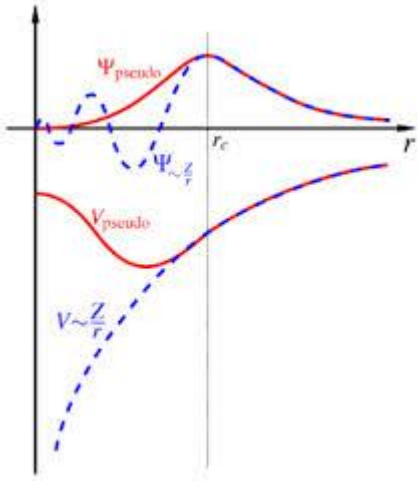
Where, ϕ_k is the pseudo wave function and ψ_κ is actual crystal wave function.

The Schrodinger equation for pseudo wave function is

$(P^2/(2m) + V_C + V_R)\,\phi_k = E\phi_k$

Where, the energy Eigen value E is same as that of real wave function.

Here, $V_R = \sum_t [(E-E_t)\langle \Phi_{k,t} / \phi_k \rangle \Phi_{k,t}\ ] / \phi_k$, which is a repulsive potential.



The figure shows both the pseudo potential and real ionic potential and their corresponding wave functions.

However, we can approximate the pseudo potential inside the core region as a constant and similar to ionic potential in interstitial regions. The Fourier transform of this potential is inversely proportional to square of the wave vectors. So, only Fourier components of reciprocal lattice vectors having smaller magnitude have to be considered.

The Schrodinger wave equation for crystal was written in matrix form and solved using the symmetric and antisymmetric form factors found in literature.

TB-LMTO-ASA method:

TB stands for tight binding and LMTO stands for linear muffin tin potential. ASA stands for atomic sphere approximation.

Muffin tin potential is defined as
U(r)= V(r-R), in core region.
U(r)= 0 , in interstitial region.

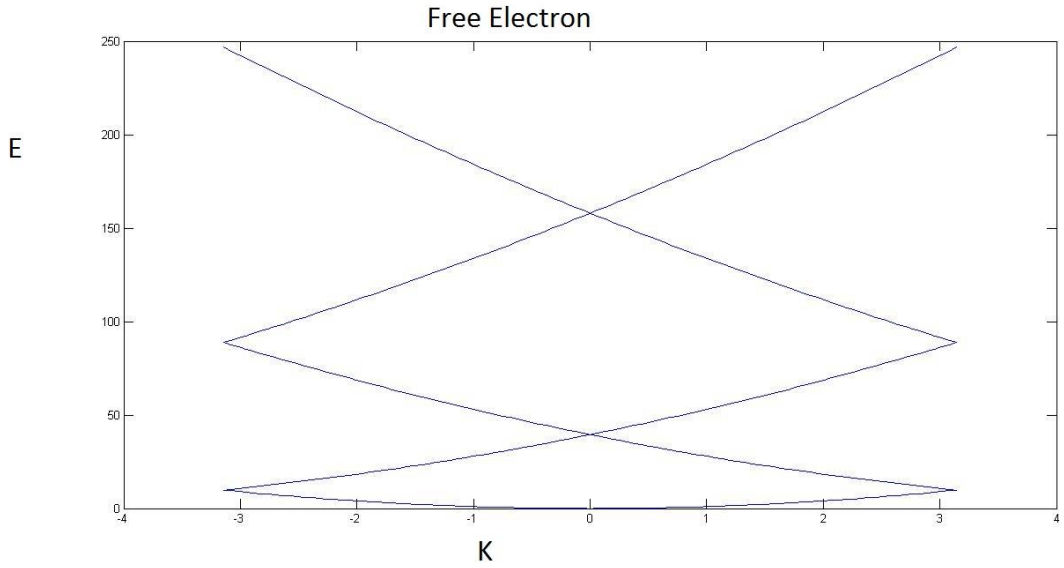
The scheme is based on the combination of the tight binding linear muffin-tin orbital (TB LMTO) method and the Real Space Green's-function.

Results

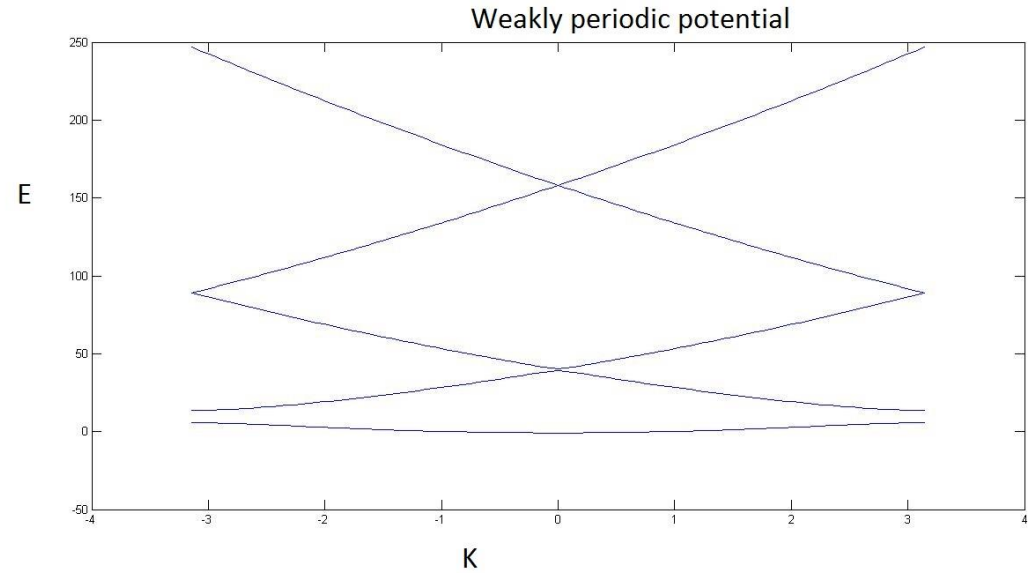
Energy vs wave vector dispersion relation of electron in weakly periodic potential:

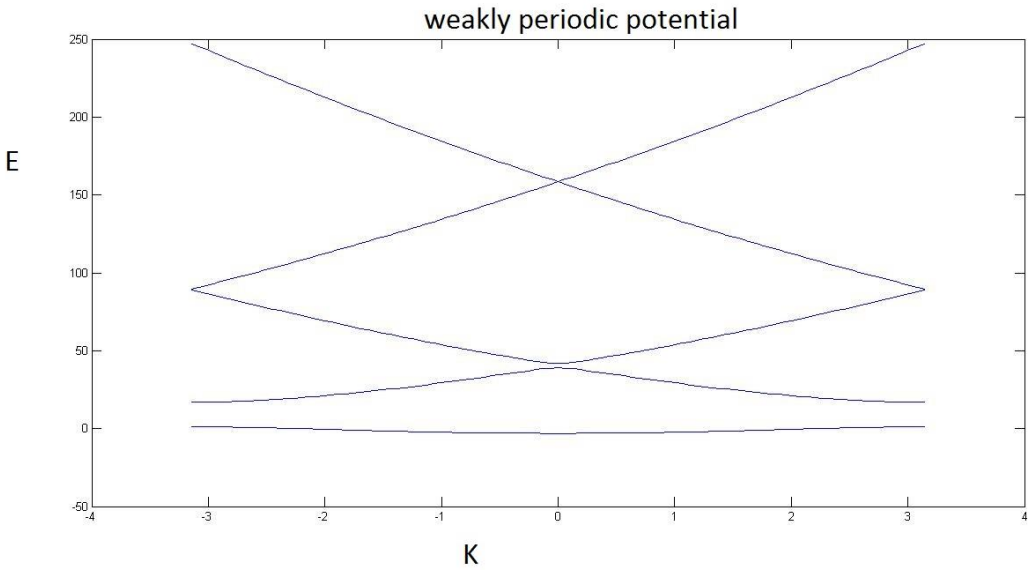
The energy vs wave vector dispersion relation of electron in a weakly periodic potential was found by writing the crystal Hamiltonian in matrix form and solving the energy Eigen values.

For free electron, the potential parameter is taken to be zero and the dispersion relation was obtained in the first brillouin zone for a one dimensional lattice in unit of ($h^2/8pi^2m$).



In a weakly periodic potential or nearly free electron model, the potential is non-zero, however, since it is weak, only fourier component smallest reciprocal lattice vectror was taken into account i.e. a small perturbation. So, dispersion curve remains nearly same, however changes near the brillouin zone due to small band gap arises.





1. Band structures of semiconductors by pseudo potential method:

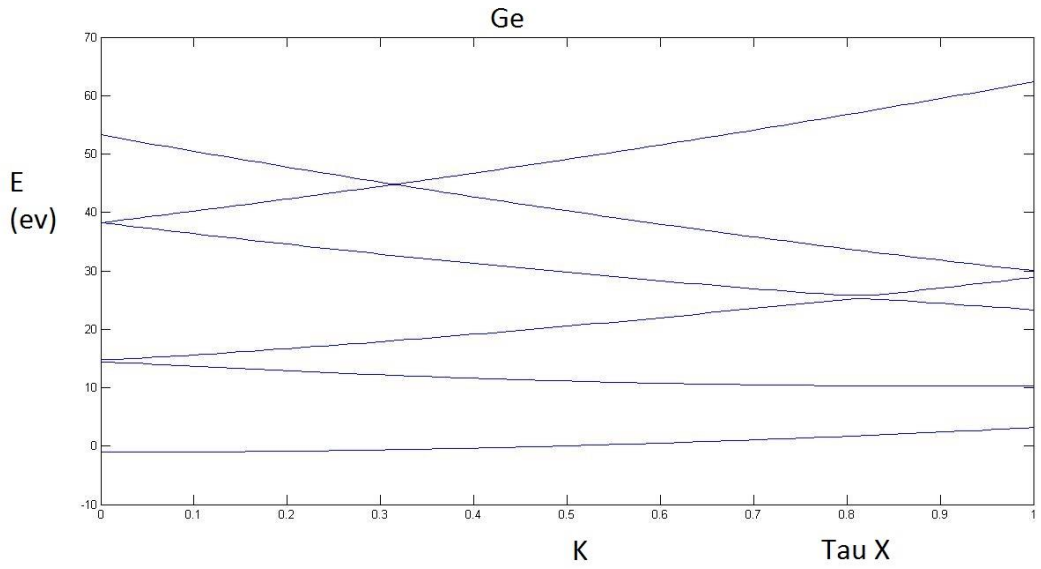
Using pseudo potential method, the band structures of various semiconductors were obtained by taking form factors for the materials from literature and was confirmed that they are semiconductors.

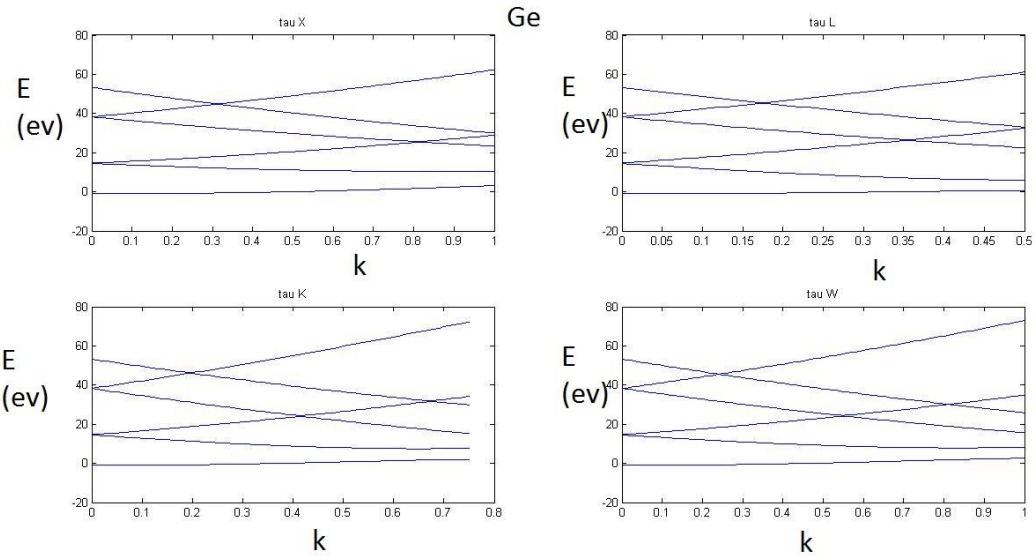
Form factor :(in Rydberg): Found in literature

Form Factor	Ge	GaAs	AlAs
V_S^3	-.23	-.23	-.221
V_S^8	.01	.01	.025
V_S^{11}	.06	.06	.07
V_A^3	0	.07	.08
V_A^4	0	.05	.05
V_A^{11}	0	.01	-.004

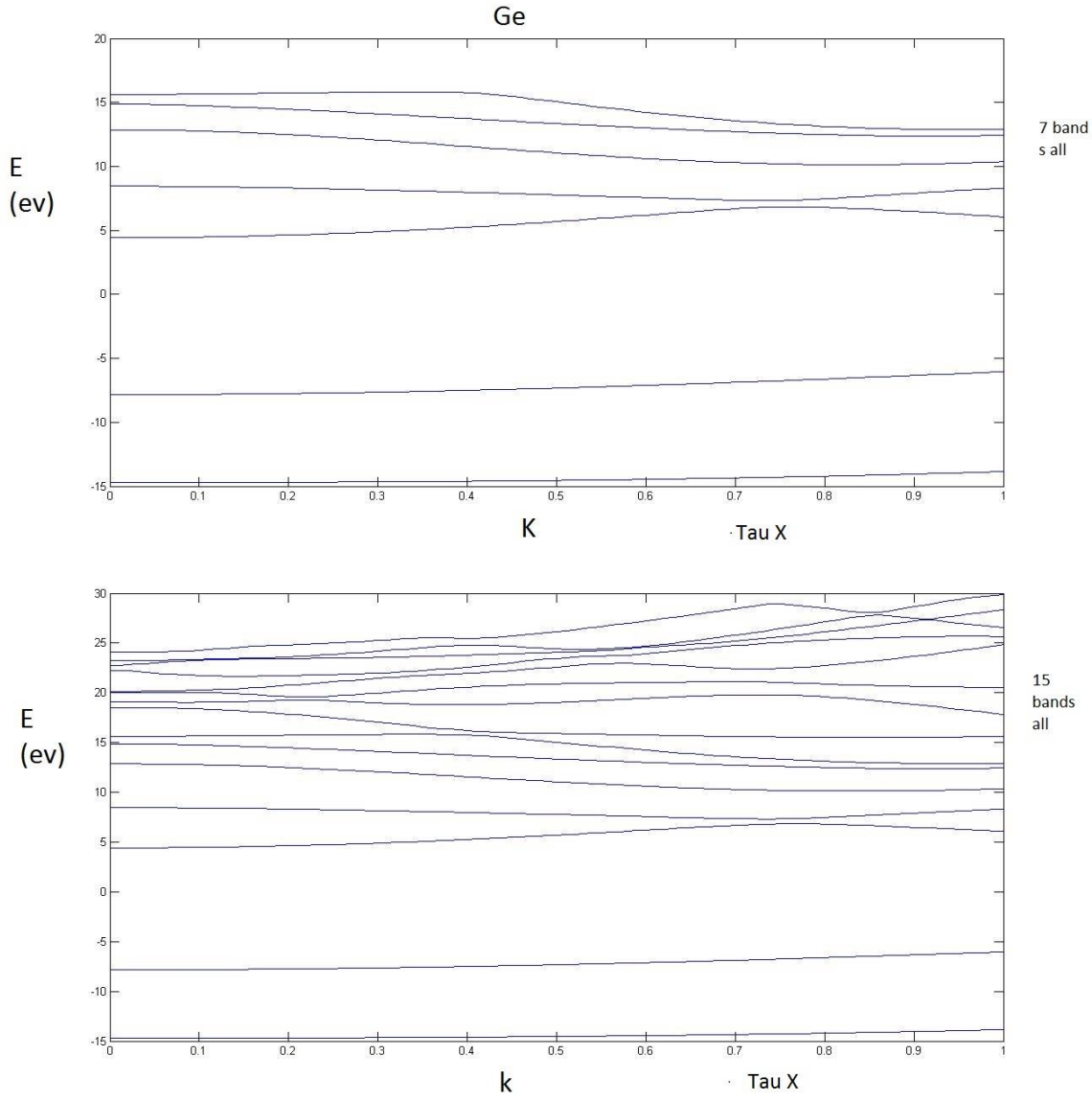
Germanium:

The band structures were plotted for germanium along different principal symmetry directions in first brillouin zone. It reveals that it is a semiconductor since the band gap is few electron volts.





Increasing the number of plane waves, more accurate result was obtained.



Matlab code to get bands for Germanium :

```
% pseudo potential for Germanium along tau X 1Ry =13.605698066 ev  v3= -
3.766ev,
% v8=0.791ev, v11= 0.2068ev
% g1=-1 1 1; g2=1 -1 1; g3=1 1 -1;g4= 1 1 1; g5= 2 0 0; g6= 0 2 0; g7= 002;
% g8=220;g9=202;g10=022;g11=2-20;g12=20-2;g13=02-2;g14=311;g15=131;g16=113;
% g17=31-1;g18=3-11;g19=13-1; g20=1-13; g21=-131;g22= -113; g23=-311;
% g24=11-3;g25=1-31
clear all
clc
a=input('enter lattice parameter in angstrom ');
h=input('enter interval length ');
b=a*10^(-10);
p=3.812*(10^(-20)); %h cross square by 2m (in ev)
g=(2*pi)/b;
k=0:h:.5;
l=0:h:.5;
m=0:h:.5;
mu=0:h:.5;
n=(.5/h)+1;
```

```
for i=1:n

    l1=p*((k(i)-1)^2+(l(i)-1)^2+(m(i)+3)^2)*g*g;
    l2=p*((k(i)-1)^2+(l(i)+3)^2+(m(i)-1)^2)*g*g;
    l3=p*((k(i)+3)^2+(l(i)-1)^2+(m(i)-1)^2)*g*g;

    l4=p*((k(i)-3)^2+(l(i)-1)^2+(m(i)+1)^2)*g*g;
    l5=p*((k(i)-3)^2+(l(i)+1)^2+(m(i)-1)^2)*g*g;
    l6=p*((k(i)-1)^2+(l(i)+1)^2+(m(i)-3)^2)*g*g;
    l7=p*((k(i)-1)^2+(l(i)-3)^2+(m(i)+1)^2)*g*g;
    l8=p*((k(i)+1)^2+(l(i)-1)^2+(m(i)-3)^2)*g*g;
    l9=p*((k(i)+1)^2+(l(i)-3)^2+(m(i)-1)^2)*g*g;

    l10=p*((k(i)-1)^2+(l(i)-1)^2+(m(i)-3)^2)*g*g;
    l11=p*((k(i)-1)^2+(l(i)-3)^2+(m(i)-1)^2)*g*g;
    l12=p*((k(i)-3)^2+(l(i)-1)^2+(m(i)-1)^2)*g*g;


   l13=p*((k(i)+0)^2+(l(i)-2)^2+(m(i)+2)^2)*g*g;
   l14=p*((k(i)-2)^2+(l(i)+0)^2+(m(i)+2)^2)*g*g;
   l15=p*((k(i)-2)^2+(l(i)+2)^2+(m(i)+0)^2)*g*g;

   l16=p*((k(i)-2)^2+(l(i)+0)^2+(m(i)-2)^2)*g*g;
   l17=p*((k(i)+0)^2+(l(i)-2)^2+(m(i)-2)^2)*g*g;
   l18=p*((k(i)-2)^2+(l(i)-2)^2+(m(i)+0)^2)*g*g;

   l19=p*((k(i)+0)^2+(l(i)+0)^2+(m(i)-2)^2)*g*g;
   l20=p*((k(i)+0)^2+(l(i)-2)^2+(m(i)+0)^2)*g*g;
   l21=p*((k(i)-2)^2+(l(i)+0)^2+(m(i)+0)^2)*g*g;

   l22=p*((k(i)-1)^2+(l(i)-1)^2+(m(i)-1)^2)*g*g;
   l23=p*((k(i)-1)^2+(l(i)-1)^2+(m(i)+1)^2)*g*g;
   l24=p*((k(i)-1)^2+(l(i)+1)^2+(m(i)-1)^2)*g*g;
   l25=p*((k(i)+1)^2+(l(i)-1)^2+(m(i)-1)^2)*g*g;


   l26=p*((k(i))^2+(l(i))^2+(m(i))^2)*g*g;

   l27=p*((k(i)-1)^2+(l(i)+1)^2+(m(i)+1)^2)*g*g;
   l28=p*((k(i)+1)^2+(l(i)-1)^2+(m(i)+1)^2)*g*g;
   l29=p*((k(i)+1)^2+(l(i)+1)^2+(m(i)-1)^2)*g*g;
   l30=p*((k(i)+1)^2+(l(i)+1)^2+(m(i)+1)^2)*g*g;

   l31=p*((k(i)+2)^2+(l(i)+0)^2+(m(i)+0)^2)*g*g;
   l32=p*((k(i)+0)^2+(l(i)+2)^2+(m(i)+0)^2)*g*g;
   l33=p*((k(i)+0)^2+(l(i)+0)^2+(m(i)+2)^2)*g*g;

   l34=p*((k(i)+2)^2+(l(i)+2)^2+(m(i)+0)^2)*g*g;
   l35=p*((k(i)+0)^2+(l(i)+2)^2+(m(i)+2)^2)*g*g;
   l36=p*((k(i)+2)^2+(l(i)+0)^2+(m(i)+2)^2)*g*g;

   l37=p*((k(i)+2)^2+(l(i)-2)^2+(m(i)+0)^2)*g*g;
   l38=p*((k(i)+2)^2+(l(i)+0)^2+(m(i)-2)^2)*g*g;
   l39=p*((k(i)+0)^2+(l(i)+2)^2+(m(i)-2)^2)*g*g;

   l40=p*((k(i)+3)^2+(l(i)+1)^2+(m(i)+1)^2)*g*g;
   l41=p*((k(i)+1)^2+(l(i)+3)^2+(m(i)+1)^2)*g*g;
   l42=p*((k(i)+1)^2+(l(i)+1)^2+(m(i)+3)^2)*g*g;

   l43=p*((k(i)-1)^2+(l(i)+3)^2+(m(i)+1)^2)*g*g;
   l44=p*((k(i)-1)^2+(l(i)+1)^2+(m(i)+3)^2)*g*g;
```

```
   l45=p*((k(i)+1)^2+(l(i)+3)^2+(m(i)-1)^2)*g*g;
   l46=p*((k(i)+1)^2+(l(i)-1)^2+(m(i)+3)^2)*g*g;
   l47=p*((k(i)+3)^2+(l(i)-1)^2+(m(i)+1)^2)*g*g;
   l48=p*((k(i)+3)^2+(l(i)+1)^2+(m(i)-1)^2)*g*g;

   l49=p*((k(i)-3)^2+(l(i)+1)^2+(m(i)+1)^2)*g*g;
   l50=p*((k(i)+1)^2+(l(i)-3)^2+(m(i)+1)^2)*g*g;
   l51=p*((k(i)+1)^2+(l(i)+1)^2+(m(i)-3)^2)*g*g;

   matrix=[l1 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791
.791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          -3.766 l2 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791
.791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          -3.766 -3.766 l3 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791
.791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          -3.766 -3.766 -3.766 l4 -3.766 -3.766 -3.766 -3.766 0 0 0 .791
.791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          -3.766 -3.766 -3.766 -3.766 l5 -3.766 -3.766 -3.766 -3.766 0 0 0
.791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          0 -3.766 -3.766 -3.766 -3.766 l6 -3.766 -3.766 -3.766 -3.766 0 0
0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          0 0 -3.766 -3.766 -3.766 -3.766 l7 -3.766 -3.766 -3.766 -3.766 0
0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          0 0 0 -3.766 -3.766 -3.766 -3.766 l8 -3.766 -3.766 -3.766 -3.766
0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l9 -3.766 -3.766 -3.766 -
3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l10 -3.766 -3.766 -
3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l11 -3.766 -
3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l12 -3.766
-3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
          .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l13 -
3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0 0 0
0;
          .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766
l14 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0 0 0
0 0;
          .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -
3.766 l15 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0 0 0 0
0 0 0;
          .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -
3.766 -3.766 l16 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791
.791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0
0 0 0 0 0 0;
          .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766
-3.766 -3.766 l17 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791
```

```
.791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 0 0 0
0 0 0 0 0 0;
          .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -
3.766 -3.766 -3.766 l18 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791
.791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
0 0 0 0 0 0 0 0;
          .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -
3.766 -3.766 -3.766 -3.766 l19 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791
.791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 0 0 0 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0
-3.766 -3.766 -3.766 -3.766 l20 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791
.791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 0 0 0 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791
0 0 0 -3.766 -3.766 -3.766 -3.766 l21 -3.766 -3.766 -3.766 -3.766 0 0 0
.791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 0 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791
.791 0 0 0 -3.766 -3.766 -3.766 -3.766 l22 -3.766 -3.766 -3.766 -3.766 0 0
0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791
.791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l23 -3.766 -3.766 -3.766 -3.766
0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791
.791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l24 -3.766 -3.766 -3.766 -
3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .791 .791
.791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l25 -3.766 -3.766 -
3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 0 0 0 0 0;
          .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .791
.791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l26 -3.766 -
3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l27 -3.766
-3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l28 -3.766
-3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l29 -3.766
-3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766 l30 -
3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766
l31 -3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766
l32 -3.766 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206;
          0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .791 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766
```

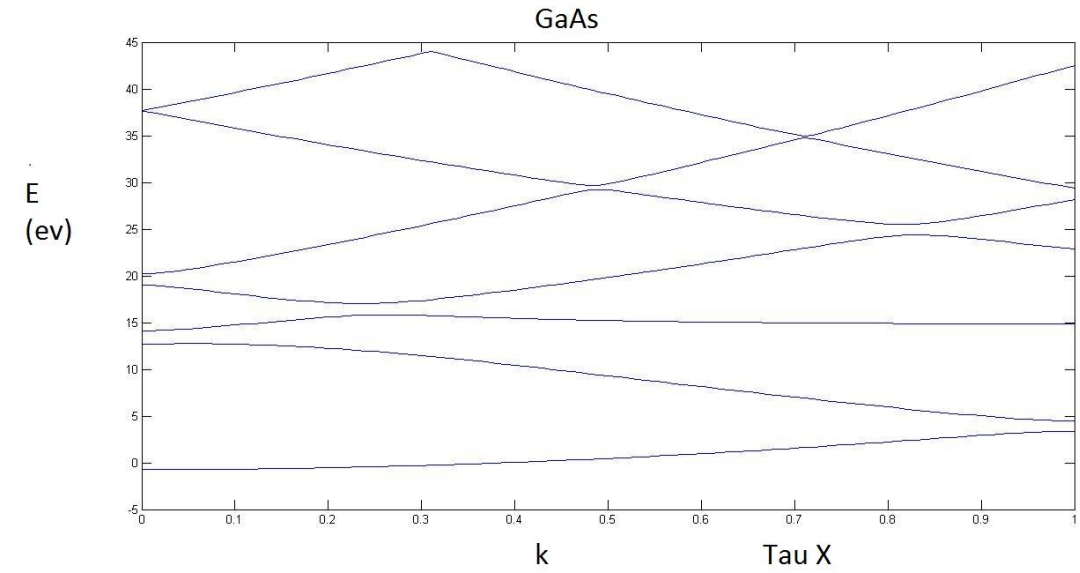
```
l33 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206
.206 .206 .206 .206;
          0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -3.766
l34 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791 .206
.206 .206 .206;
          0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -
3.766 l35 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791
.206 .206 .206;
          0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -3.766 -
3.766 l36 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791 .791
.206 .206;
          0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -
3.766 -3.766 l37 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791
.791 .206;
          0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -
3.766 -3.766 l38 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791 .791
.791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766 -
3.766 -3.766 l39 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791
.791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766
-3.766 -3.766 l40 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791 .791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -3.766
-3.766 -3.766 l41 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791 .791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -
3.766 -3.766 -3.766 l42 -3.766 -3.766 -3.766 -3.766 0 0 0 .791 .791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -
3.766 -3.766 -3.766 l43 -3.766 -3.766 -3.766 -3.766 0 0 0 .791;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -3.766 -
3.766 -3.766 -3.766 l44 -3.766 -3.766 -3.766 -3.766 0 0 0;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -
3.766 -3.766 -3.766 -3.766 l45 -3.766 -3.766 -3.766 -3.766 0 0;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0 -
3.766 -3.766 -3.766 -3.766 l46 -3.766 -3.766 -3.766 -3.766 0;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0
-3.766 -3.766 -3.766 -3.766 l47 -3.766 -3.766 -3.766 -3.766;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0
-3.766 -3.766 -3.766 -3.766 l48 -3.766 -3.766 -3.766;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791 0 0 0
-3.766 -3.766 -3.766 -3.766 l50 -3.766 -3.766;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791
0 0 0 -3.766 -3.766 -3.766 -3.766 l50 -3.766;
          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 .206 .206 .206
.206 .206 .206 .206 .206 .206 .206 .206 .206 .206 .791 .791 .791 .791 .791 .791
0 0 0 -3.766 -3.766 -3.766 -3.766 l51]

   egn=eig(matrix);
```

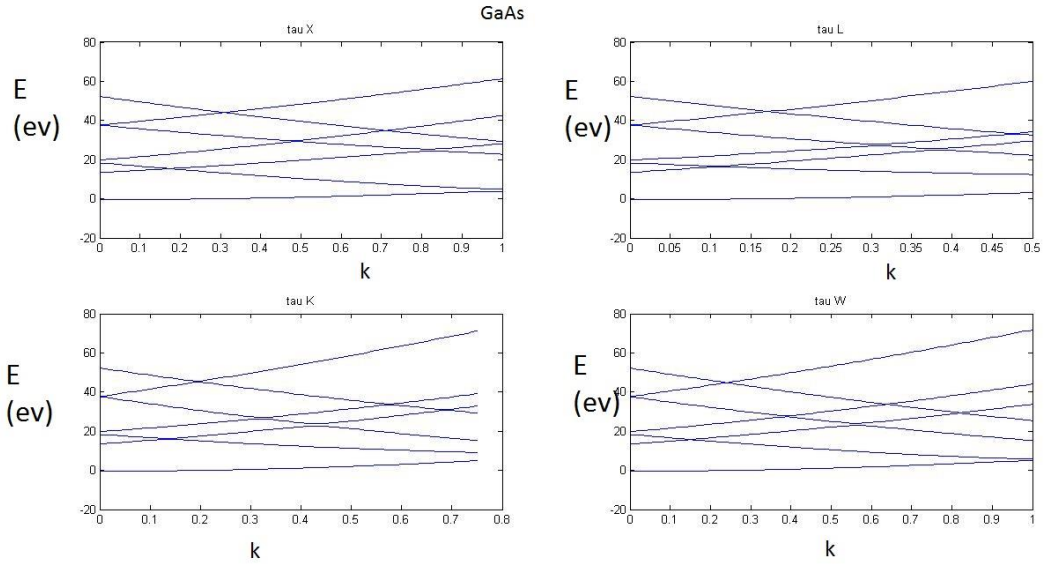
```
    e1(i)=egn(1);
    e2(i)=egn(2);
    e3(i)=egn(3);
    e4(i)=egn(4);
    e5(i)=egn(5);
    e6(i)=egn(6);
    e7(i)=egn(7);
    e8(i)=egn(8);
    e9(i)=egn(9);
    e10(i)=egn(10);

    e11(i)=egn(11);
    e12(i)=egn(12);
    e13(i)=egn(13);
    e14(i)=egn(14);
    e15(i)=egn(15);
    e16(i)=egn(16);
    e17(i)=egn(17);
    e18(i)=egn(18);
    e19(i)=egn(19);
    e20(i)=egn(20);

    e21(i)=egn(21);
    e22(i)=egn(22);
    e23(i)=egn(23);
    e24(i)=egn(24);
    e25(i)=egn(25);
    e26(i)=egn(26);
    e27(i)=egn(27);
    e28(i)=egn(28);
    e29(i)=egn(29);
    e30(i)=egn(30);

    e31(i)=egn(31);
    e32(i)=egn(32);
    e33(i)=egn(33);
    e34(i)=egn(34);
    e35(i)=egn(35);
    e36(i)=egn(36);
    e37(i)=egn(37);
    e38(i)=egn(38);
    e39(i)=egn(39);
    e40(i)=egn(40);

    e41(i)=egn(41);
    e42(i)=egn(42);
    e43(i)=egn(43);
    e44(i)=egn(44);
    e45(i)=egn(45);
    e46(i)=egn(46);
    e47(i)=egn(47);
    e48(i)=egn(48);
    e49(i)=egn(49);
    e50(i)=egn(50);
    e51(i)=egn(51);

end

plot(mu,e1)
hold on
plot(mu,e2)
```

```
hold on
plot(mu,e3)
hold on
plot(mu,e4)
hold on
plot(mu,e5)
hold on
plot(mu,e6)
hold on
plot(mu,e7)
hold on
plot(mu,e8)
hold on
plot(mu,e9)
hold on

plot(mu,e10)
hold on
plot(mu,e11)
hold on
plot(mu,e12)
hold on
plot(mu,e13)
hold on
plot(mu,e14)
hold on
plot(mu,e15)
```

1.1Gallium arsenide:

Similarly, the band plots were obtained for gallium arsenide along different principal symmetry directions in the first brillouin zone which reveals that it is direct band gap semiconductor.





Matlab code to get bands of Gallium Arsenide along different crystallographic directions using lesser number of Fourier components:

```
%pseudo potential for GaAs
 %along tau X and tau L 1Ry =13.605698066 ev  v3= -3.766ev,
% v8=0.791ev, v11= 0.2068ev
% Fourier components, v3=2.662ev, v8=-.791, v11=-.146 (important)
clear all
clc
a=input('enter lattice parameter in angstrom ');
h=input('enter interval length ');
b=a*10^(-10);
p=3.812*(10^(-20)); %h cross square by 2m (in ev)
g=(2*pi)/b;

%  TAU X
k1=0:h:1;
mu1=0:h:1;
n=(1/h)+1;
for i=1:n
    l1(i)=0;
    m1(i)=0;
end

for i=1:n
```

```
   l11=p*g^2*((k1(i)-3)^2+(l1(i)-1)^2+(m1(i)-1)^2);
   l21=p*g^2*((k1(i)-2)^2+(l1(i)-2)^2+(m1(i)-0)^2);
   l31=p*g^2*((k1(i)-2)^2+(l1(i)-0)^2+(m1(i)-0)^2);
   l41=p*g^2*((k1(i)-1)^2+(l1(i)-1)^2+(m1(i)-1)^2);

   l51=p*g^2*((k1(i))^2+(l1(i))^2+(m1(i))^2);

   l61=p*g^2*((k1(i)+1)^2+(l1(i)+1)^2+(m1(i)+1)^2);
   l71=p*g^2*((k1(i)+2)^2+(l1(i)+0)^2+(m1(i)+0)^2);
   l81=p*g^2*((k1(i)+2)^2+(l1(i)+2)^2+(m1(i)+0)^2);
   l91=p*g^2*((k1(i)+3)^2+(l1(i)+1)^2+(m1(i)+1)^2);

   matrix1=[l11 2.212-.673i -.680i -.136 -.576+.096i 0 0 0 0;
          2.212+.673i l21 2.212-.673i -.680i -.136 -.576+.096i 0 0 0;
          .680i 2.212+.673i l31 2.212-.673i -.680i -.136 -.576+.096i 0 0;
          -.136 .680i 2.212+.673i 141 2.212-.673i -.680i -.136 -.576+.096i
0;
          -.576-.096i -.136 .680i 2.212+.673i l51 2.212-.673i -.680i -.136
-.576+.096i;
          0 -.576-.096i -.136 .680i 2.212+.673i l61 2.212-.673i -.680i -
.136;
          0 0 -.576-.096i -.136 .680i 2.212+.673i l71 2.212-.673i -.680i;
          0 0 0 -.576-.096i -.136 .680i 2.212+.673i l81 2.212-.673i;
          0 0 0 0 -.576-.096i -.136 .680i 2.212+.673i l91];

   egn1=eig(matrix1);
   e11(i)=egn1(1);
   e21(i)=egn1(2);
   e31(i)=egn1(3);
   e41(i)=egn1(4);
   e51(i)=egn1(5);
   e61(i)=egn1(6);
   e71(i)=egn1(7);
end
  subplot(2,2,1),
plot(mu1,e11)
hold on
plot(mu1,e21)
hold on
plot(mu1,e31)
hold on
plot(mu1,e41)
hold on
plot(mu1,e51)
hold on
plot(mu1,e61)

title('tau X')
% tau L

k2=0:h:.5;
l2=0:h:.5;
m2=0:h:.5;
mu2=0:h:.5;
n=(.5/h)+1;
for i=1:n
   l12=p*g^2*((k2(i)-3)^2+(l2(i)-1)^2+(m2(i)-1)^2);
   l22=p*g^2*((k2(i)-2)^2+(l2(i)-2)^2+(m2(i)-0)^2);
   l32=p*g^2*((k2(i)-2)^2+(l2(i)-0)^2+(m2(i)-0)^2);
   l42=p*g^2*((k2(i)-1)^2+(l2(i)-1)^2+(m2(i)-1)^2);

   l52=p*g^2*((k2(i))^2+(l2(i))^2+(m2(i))^2);
```

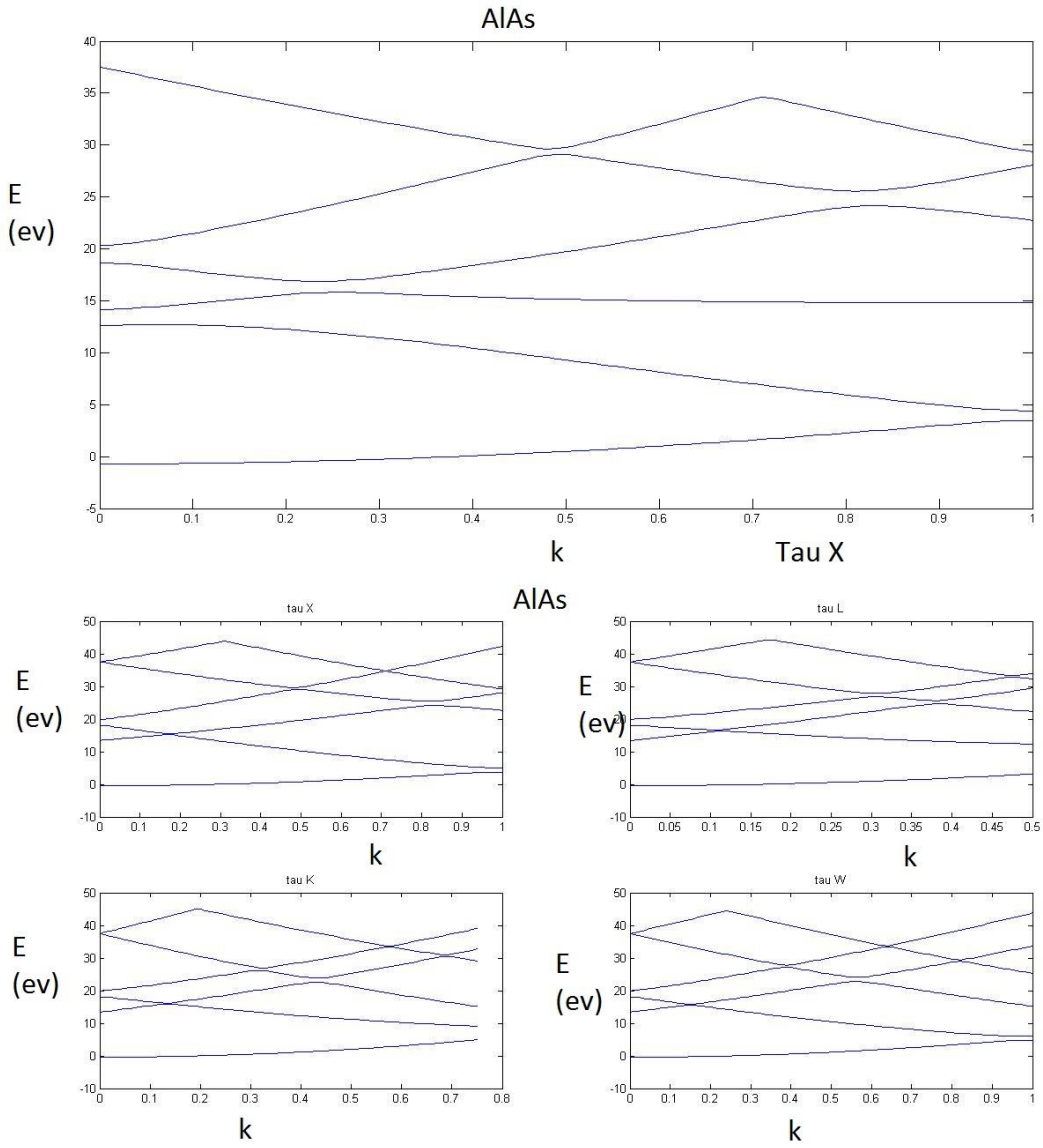
```
   l62=p*g^2*((k2(i)+1)^2+(l2(i)+1)^2+(m2(i)+1)^2);
   l72=p*g^2*((k2(i)+2)^2+(l2(i)+0)^2+(m2(i)+0)^2);
   l82=p*g^2*((k2(i)+2)^2+(l2(i)+2)^2+(m2(i)+0)^2);
   l92=p*g^2*((k2(i)+3)^2+(l2(i)+1)^2+(m2(i)+1)^2);

   matrix2=[l12 2.212-.673i -.680i -.136 -.576+.096i 0 0 0 0;
          2.212+.673i l22 2.212-.673i -.680i -.136 -.576+.096i 0 0 0;
          .680i 2.212+.673i l32 2.212-.673i -.680i -.136 -.576+.096i 0 0;
          -.136 .680i 2.212+.673i 142 2.212-.673i -.680i -.136 -.576+.096i
0;
          -.576-.096i -.136 .680i 2.212+.673i l52 2.212-.673i -.680i -.136
-.576+.096i;
          0 -.576-.096i -.136 .680i 2.212+.673i l62 2.212-.673i -.680i -
.136;
          0 0 -.576-.096i -.136 .680i 2.212+.673i l72 2.212-.673i -.680i;
          0 0 0 -.576-.096i -.136 .680i 2.212+.673i l82 2.212-.673i;
          0 0 0 0 -.576-.096i -.136 .680i 2.212+.673i l92];

   egn2=eig(matrix2);
   e12(i)=egn2(1);
   e22(i)=egn2(2);
   e32(i)=egn2(3);
   e42(i)=egn2(4);
   e52(i)=egn2(5);
   e62(i)=egn2(6);
   e72(i)=egn2(7);

end
  subplot(2,2,2),
plot(mu2,e12)
hold on
plot(mu2,e22)
hold on
plot(mu2,e32)
hold on
plot(mu2,e42)
hold on
plot(mu2,e52)
hold on
plot(mu2,e62)

title('tau L')
% tau K

k3=0:h:.75;
l3=0:h:.75;
mu3=0:h:.75;
n=(.75/h)+1;
for i=1:n
    m3(i)=0;
end
for i=1:n
   l13=p*g^2*((k3(i)-3)^2+(l3(i)-1)^2+(m3(i)-1)^2);
   l23=p*g^2*((k3(i)-2)^2+(l3(i)-2)^2+(m3(i)-0)^2);
   l33=p*g^2*((k3(i)-2)^2+(l3(i)-0)^2+(m3(i)-0)^2);
   l43=p*g^2*((k3(i)-1)^2+(l3(i)-1)^2+(m3(i)-1)^2);

   l53=p*g^2*((k3(i))^2+(l3(i))^2+(m3(i))^2);

   l63=p*g^2*((k3(i)+1)^2+(l3(i)+1)^2+(m3(i)+1)^2);
   l73=p*g^2*((k3(i)+2)^2+(l3(i)+0)^2+(m3(i)+0)^2);
   l83=p*g^2*((k3(i)+2)^2+(l3(i)+2)^2+(m3(i)+0)^2);
   l93=p*g^2*((k3(i)+3)^2+(l3(i)+1)^2+(m3(i)+1)^2);
```

```
   matrix3=[l13 2.212-.673i -.680i -.136 -.576+.096i 0 0 0 0;
          2.212+.673i l23 2.212-.673i -.680i -.136 -.576+.096i 0 0 0;
          .680i 2.212+.673i l33 2.212-.673i -.680i -.136 -.576+.096i 0 0;
          -.136 .680i 2.212+.673i 143 2.212-.673i -.680i -.136 -.576+.096i
0;
          -.576-.096i -.136 .680i 2.212+.673i l53 2.212-.673i -.680i -.136
-.576+.096i;
          0 -.576-.096i -.136 .680i 2.212+.673i l63 2.212-.673i -.680i -
.136;
          0 0 -.576-.096i -.136 .680i 2.212+.673i l73 2.212-.673i -.680i;
          0 0 0 -.576-.096i -.136 .680i 2.212+.673i l83 2.212-.673i;
          0 0 0 0 -.576-.096i -.136 .680i 2.212+.673i l93];

   egn3=eig(matrix3);
   e13(i)=egn3(1);
   e23(i)=egn3(2);
   e33(i)=egn3(3);
   e43(i)=egn3(4);
   e53(i)=egn3(5);
   e63(i)=egn3(6);
   e73(i)=egn3(7);

end
  subplot(2,2,3),
plot(mu3,e13)
hold on
plot(mu3,e23)
hold on
plot(mu3,e33)
hold on
plot(mu3,e43)
hold on
plot(mu3,e53)
hold on
plot(mu3,e63)

title('tau K')
% tau W

k4=0:h:1;
l4=0:h:1;
mu4=0:h:1;
n=(1/h)+1;
for i=1:n
    m4(i)=0;
end
for i=1:n
   l14=p*g^2*((k4(i)-3)^2+(l4(i)*.5-1)^2+(m4(i)-1)^2);
   l24=p*g^2*((k4(i)-2)^2+(l4(i)*.5-2)^2+(m4(i)-0)^2);
   l34=p*g^2*((k4(i)-2)^2+(l4(i)*.5-0)^2+(m4(i)-0)^2);
   l44=p*g^2*((k4(i)-1)^2+(l4(i)*.5-1)^2+(m4(i)-1)^2);

   l54=p*g^2*((k4(i))^2+(l4(i)*.5)^2+(m4(i))^2);

   l64=p*g^2*((k4(i)+1)^2+(l4(i)*.5+1)^2+(m4(i)+1)^2);
   l74=p*g^2*((k4(i)+2)^2+(l4(i)*.5+0)^2+(m4(i)+0)^2);
   l84=p*g^2*((k4(i)+2)^2+(l4(i)*.5+2)^2+(m4(i)+0)^2);
   l94=p*g^2*((k4(i)+3)^2+(l4(i)*.5+1)^2+(m4(i)+1)^2);

   matrix4=[l14 2.212-.673i -.680i -.136 -.576+.096i 0 0 0 0;
          2.212+.673i l24 2.212-.673i -.680i -.136 -.576+.096i 0 0 0;
          .680i 2.212+.673i l34 2.212-.673i -.680i -.136 -.576+.096i 0 0;
```

```
          -.136 .680i 2.212+.673i 144 2.212-.673i -.680i -.136 -.576+.096i
0;
          -.576-.096i -.136 .680i 2.212+.673i l54 2.212-.673i -.680i -.136
-.576+.096i;
          0 -.576-.096i -.136 .680i 2.212+.673i l64 2.212-.673i -.680i -
.136;
          0 0 -.576-.096i -.136 .680i 2.212+.673i l74 2.212-.673i -.680i;
          0 0 0 -.576-.096i -.136 .680i 2.212+.673i l84 2.212-.673i;
          0 0 0 0 -.576-.096i -.136 .680i 2.212+.673i l94];

   egn4=eig(matrix4);
   e14(i)=egn4(1);
   e24(i)=egn4(2);
   e34(i)=egn4(3);
   e44(i)=egn4(4);
   e54(i)=egn4(5);
   e64(i)=egn4(6);
   e74(i)=egn4(7);

end
  subplot(2,2,4),
plot(mu4,e14)
hold on
plot(mu4,e24)
hold on
plot(mu4,e34)
hold on
plot(mu4,e44)
hold on
plot(mu4,e54)
hold on
plot(mu4,e64)
title('tau W')
```

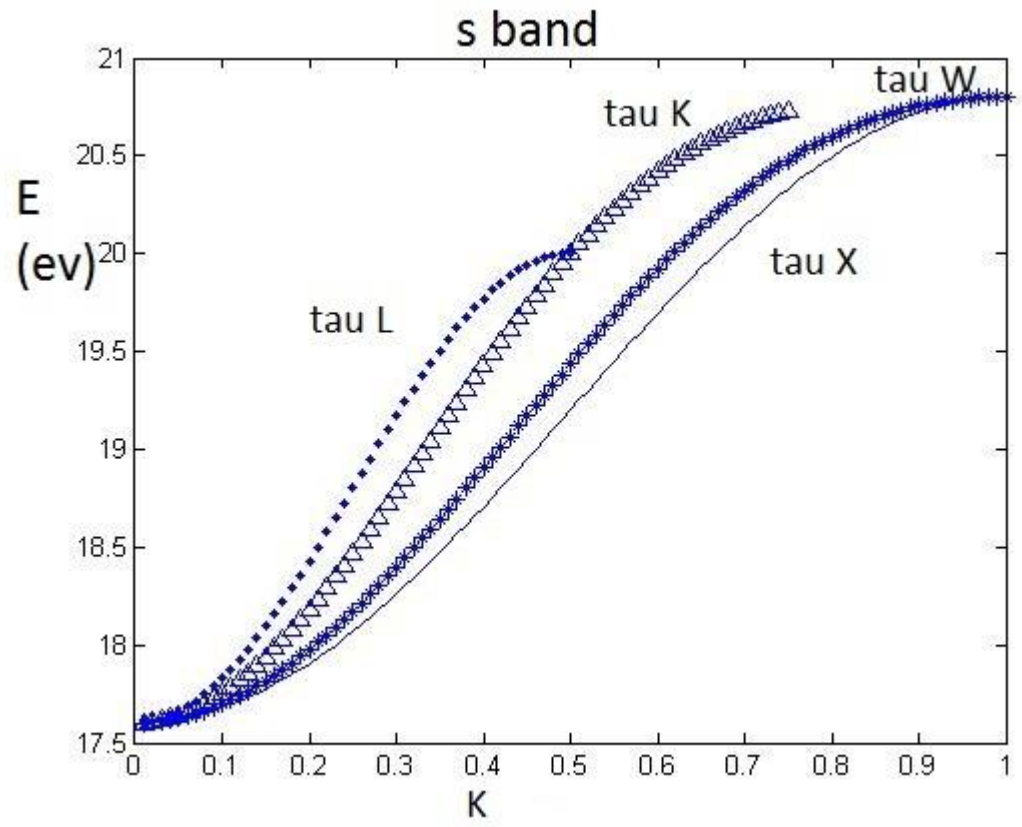
Aluminium arsenide (AlAs):

Similarly, the band plots were obtained for aluminium arsenide along different principal symmetry directions in the first brillouin zone which reveals that it is semiconductor.

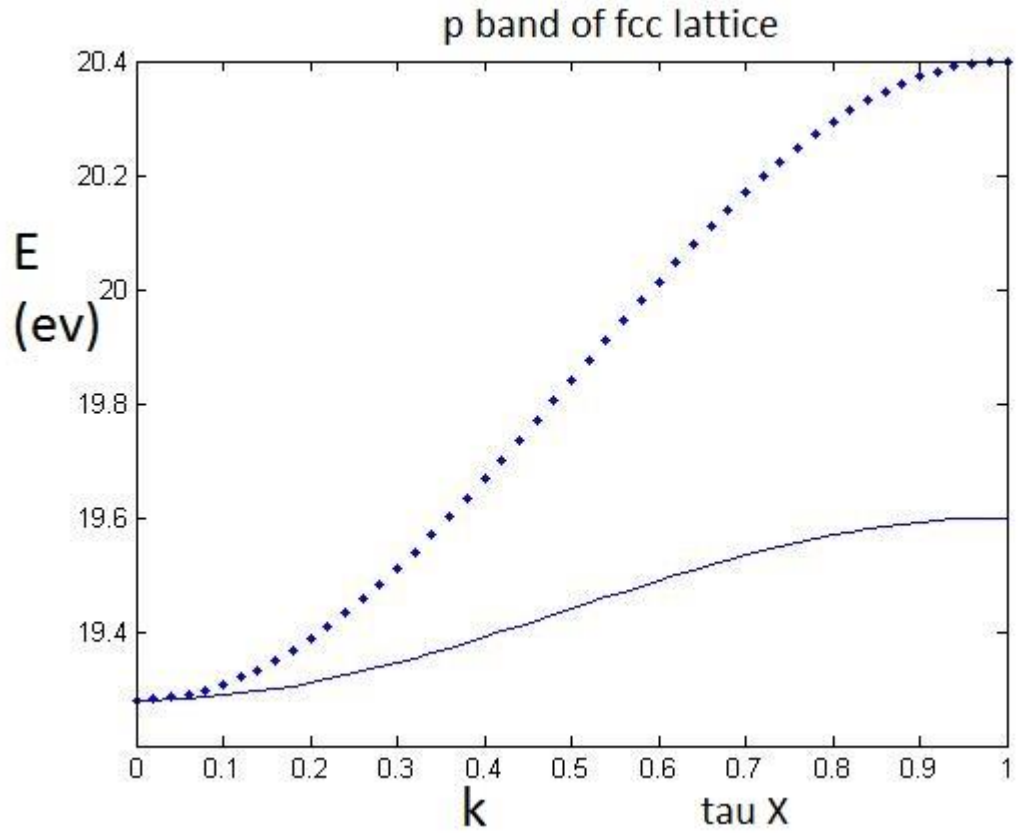


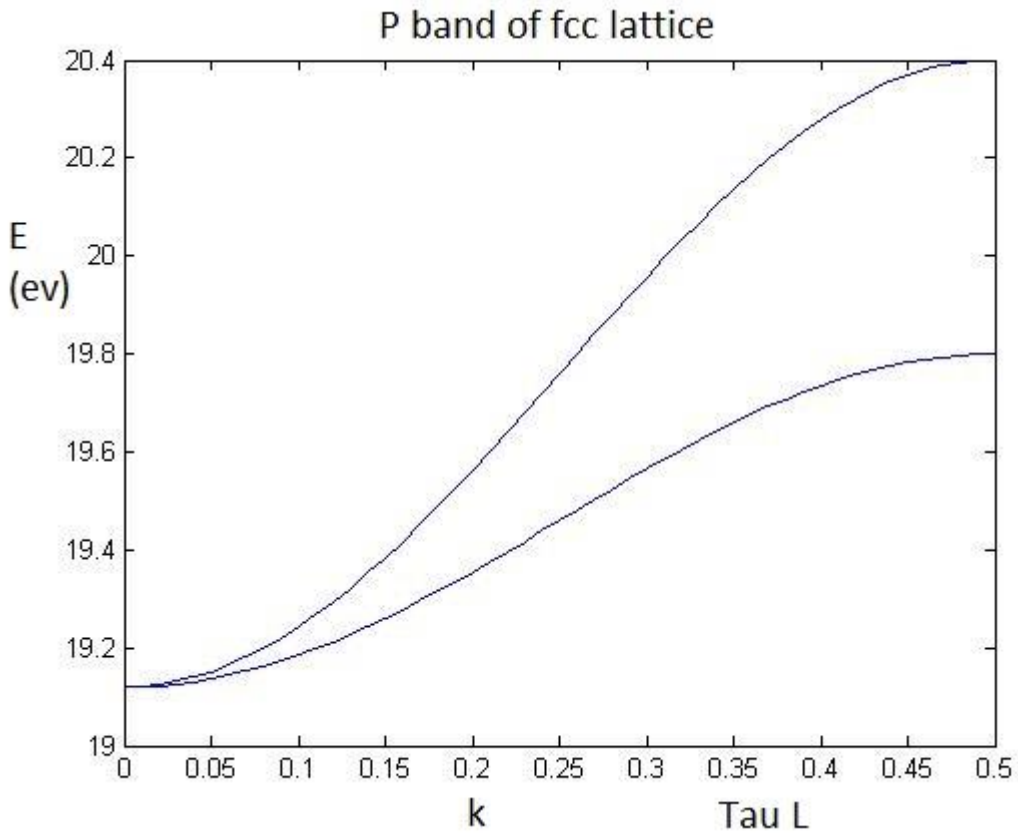
Tight binding method:

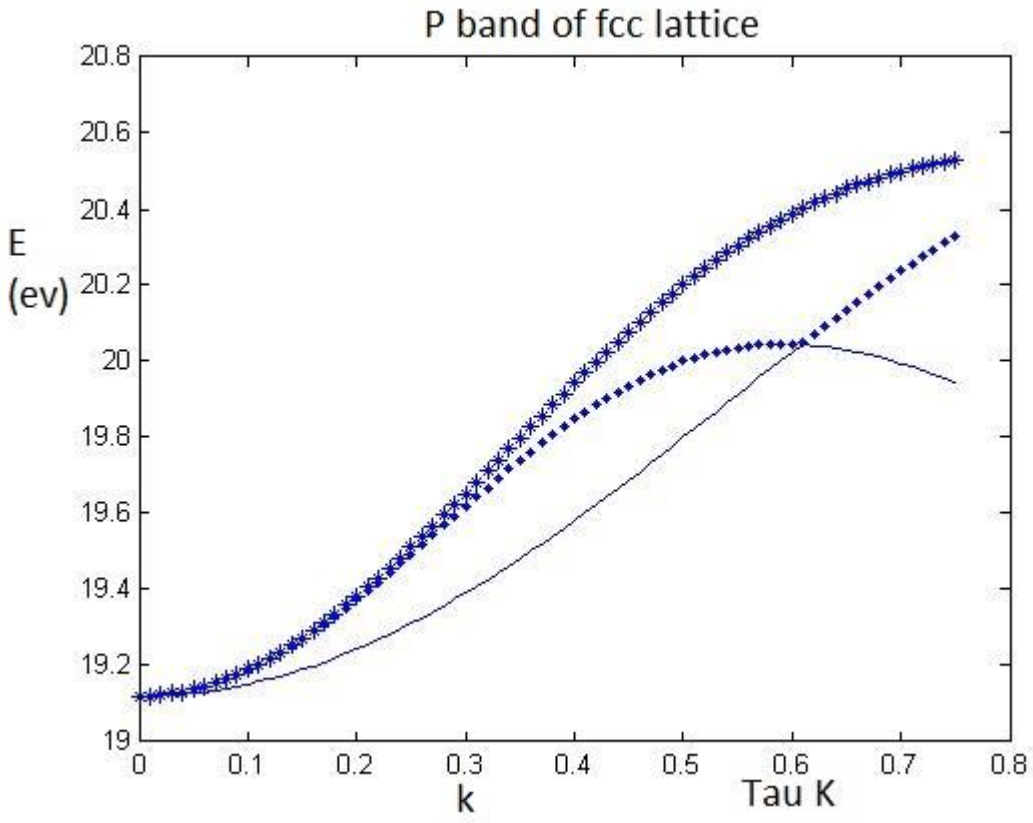
Tight binding method was applied to get s-band of a face centred cubic lattice was along principal symmetry directions in the first brillouin zone.



Similarly, the tight binding method was applied to get the p-bands using degenerate atomic p orbitals as unperturbed wave functions.
The p energy bands were plotted along different principal symmetry directions. It was found that the p bands are doubly degenerate along Γ X and Γ L directions.


p band of fcc lattice
E
(ev)
20.4
20.2
20
19.8
19.6
19.4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
k
tau X


P band of fcc lattice
E
(ev)
20.4
20.2
20
19.8
19.6
19.4
19.2
19
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
k
Tau L



Electronic properties of III-V semiconductor and its superlattices by TB- LMTO code:

List of programs in TB-LMTO-ASA to get band structures and density of states.:

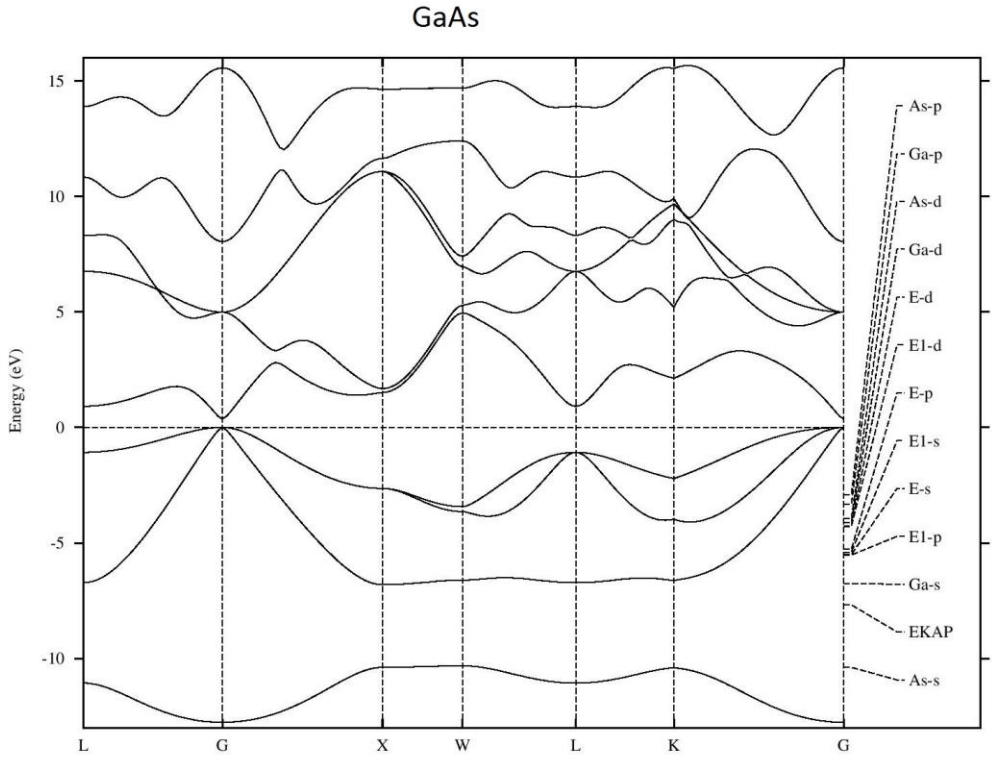
1) ../lminit.run
2) ../ lmhart.run
3) ../lmovl.run
4) ../lmes.run
5) ../lmovl.run
6) ../lmctl.run
7) ../lmstr.run
8) ../lm.run
9) ../lm.run
10) ../lm.run
11) ../lmbnd.run
12) ../gnubnd.run
13) gnuplot BNDS.GNU
14) ../lmdos.run
15) ../gnudos.run
16) gnuplot DOS.GNU

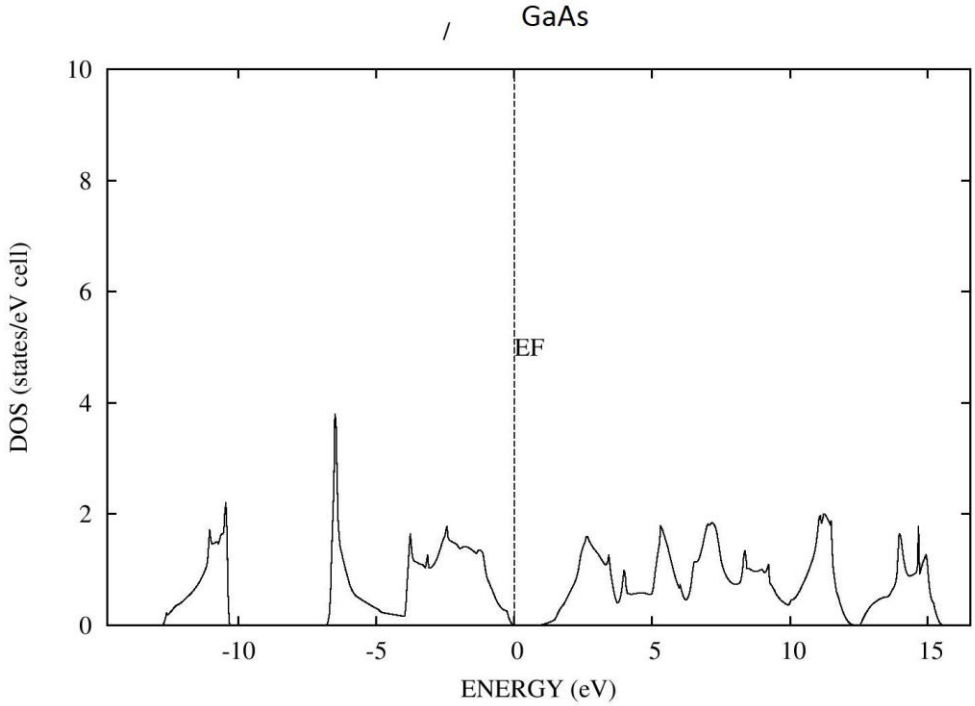
The constituent atoms, its lattice positions and the space group of the material was given as input to find the respective band structures and density of states

Gallium Arsenide (GaAs):

The lattice position of Ga is (0,0,0) and position of As is (.25,.25,.25). the band structure predicts that its band gap is nearly 1.5ev which lies on the same wave vector. so it is a direct band gap semiconductor.

The density of states vanishes between -10ev to -6ev energy and also vanishes near 0ev energy. The density of states spreads up to 15ev since the bands exist up to that energy range.

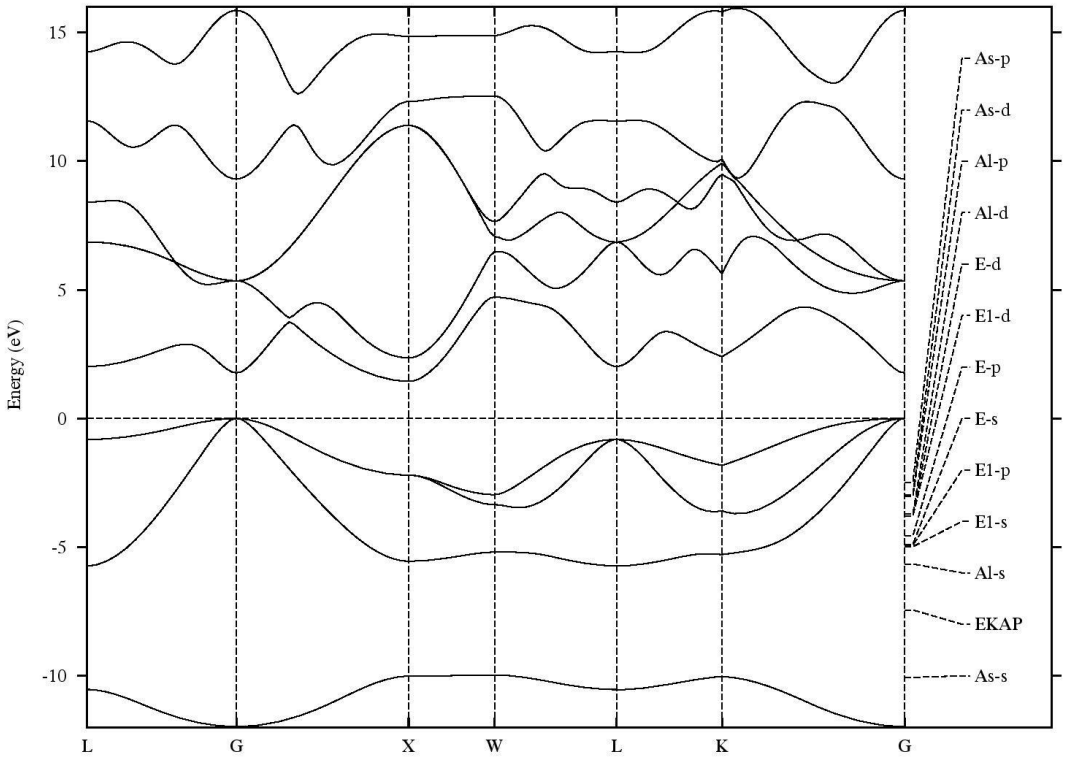




Aluminium arsenide:

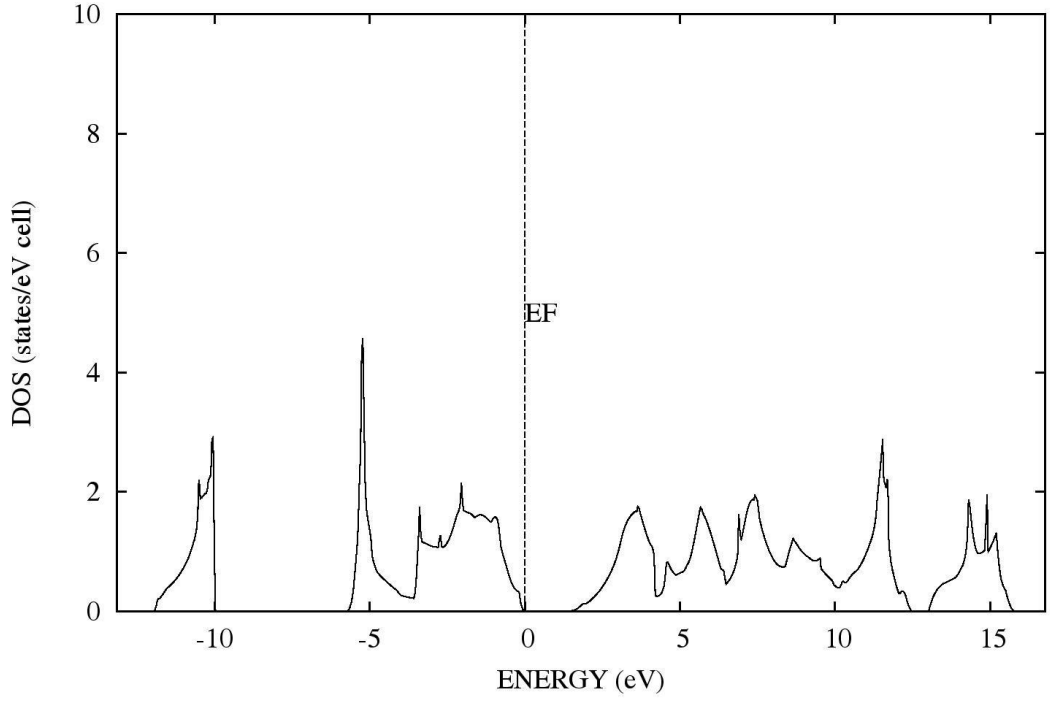
The band structure reveals that its band gap lies in the range of nearly 2ev. So, it is a semiconductor.

AlAs


15
10
5
0
-5
-10
Energy (eV)
L
G
X
W
L
K
G
As-p
As-d
Al-p
Al-d
E-d
E1-d
E-p
E-s
E1-p
E1-s
Al-s
EKAP
As-s

AlAs

/

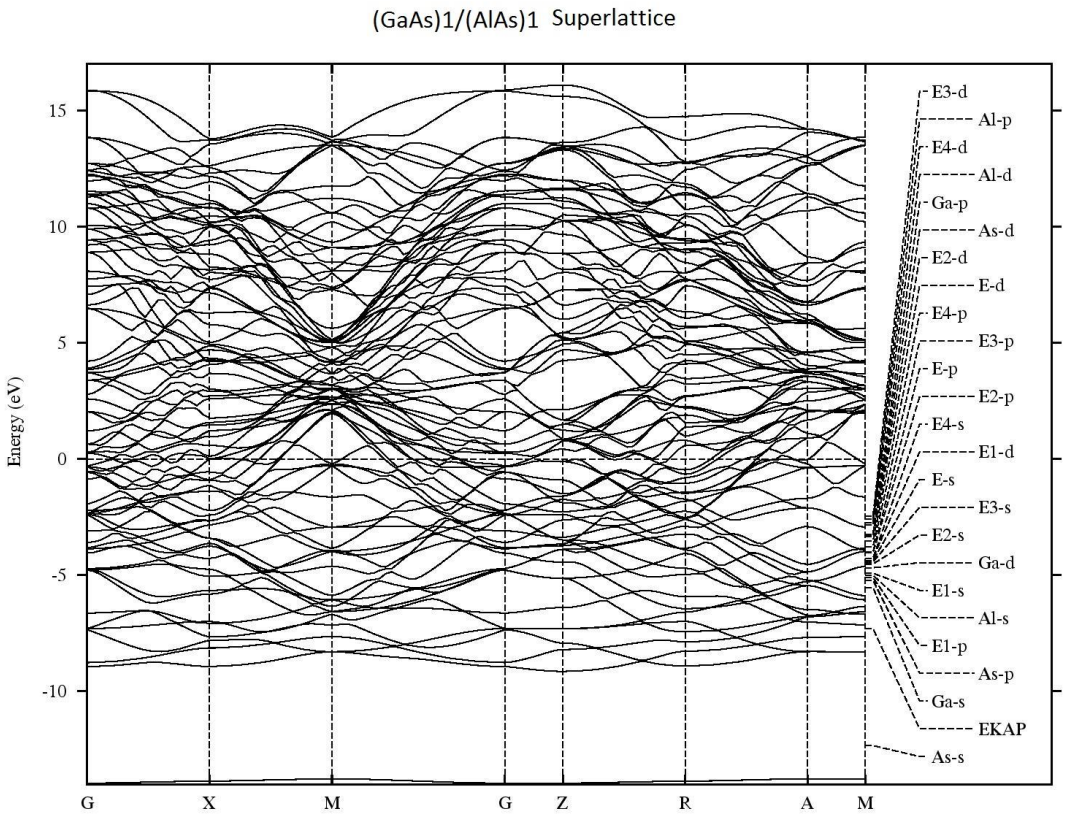

10
8
6
4
2
0
DOS (states/eV cell)
EF
-10
-5
0
5
10
15
ENERGY (eV)

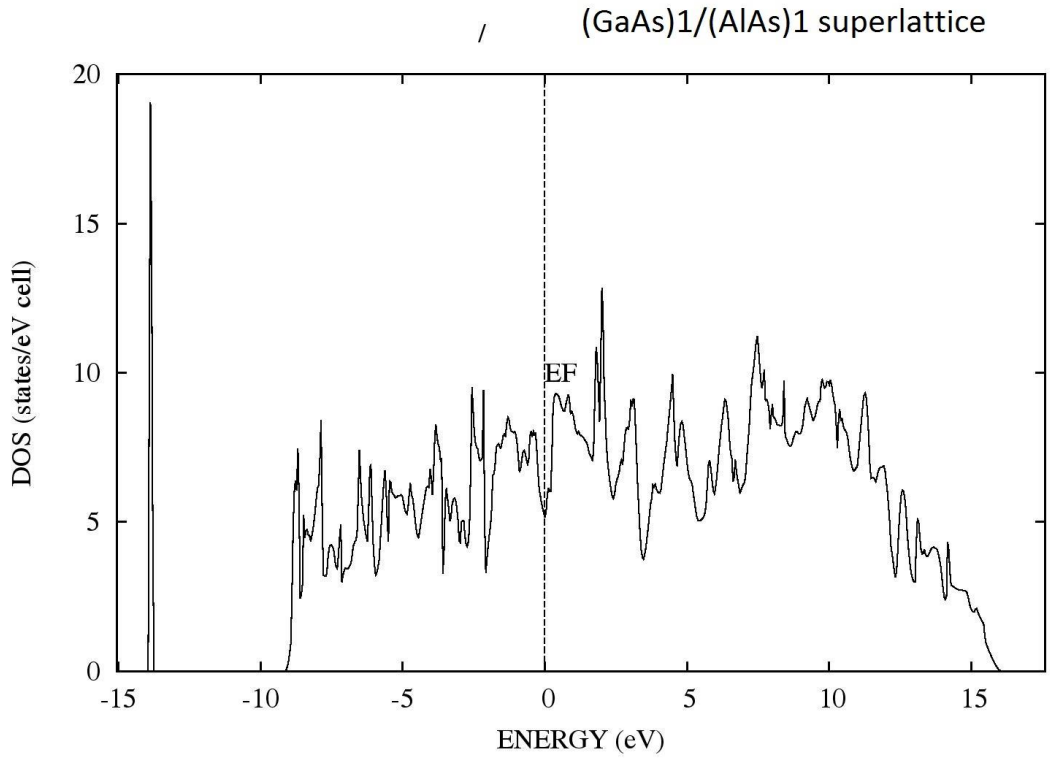
$(GaAs)_1/(AlAs)_1$ superlattice:

Its period is twice that of its single crystals. Its period consists of one unit cell of gallium arsenide and one unit cell of aluminium arsenide.The $(GaAs)_1/(AlAs)_1$ superlattice was grown along (001) direction of crystallographic axes. The lattice constants of two materials are nearly same and vary by .15%. so, there is no strain in this, hence it has advantage compared to other materials.

The band structure and density of states of this superlattice were plotted using TB-LMTO code. The band structure predicts that the minibands or subbands have been formed and forbidden gaps between consecutive bands have become narrow. This is due to the extended periodicity of superlattice along the growth direction. The density of states shows it is continuous and have high value compared to its single crystals counterpart within the specified energy range. The density of states drops to zero above 15ev.This is obvious since more number of bands are present in superlattices than the single crystal due to its extended periodicity.

So, the electronic properties have significantly changed in superlattice.



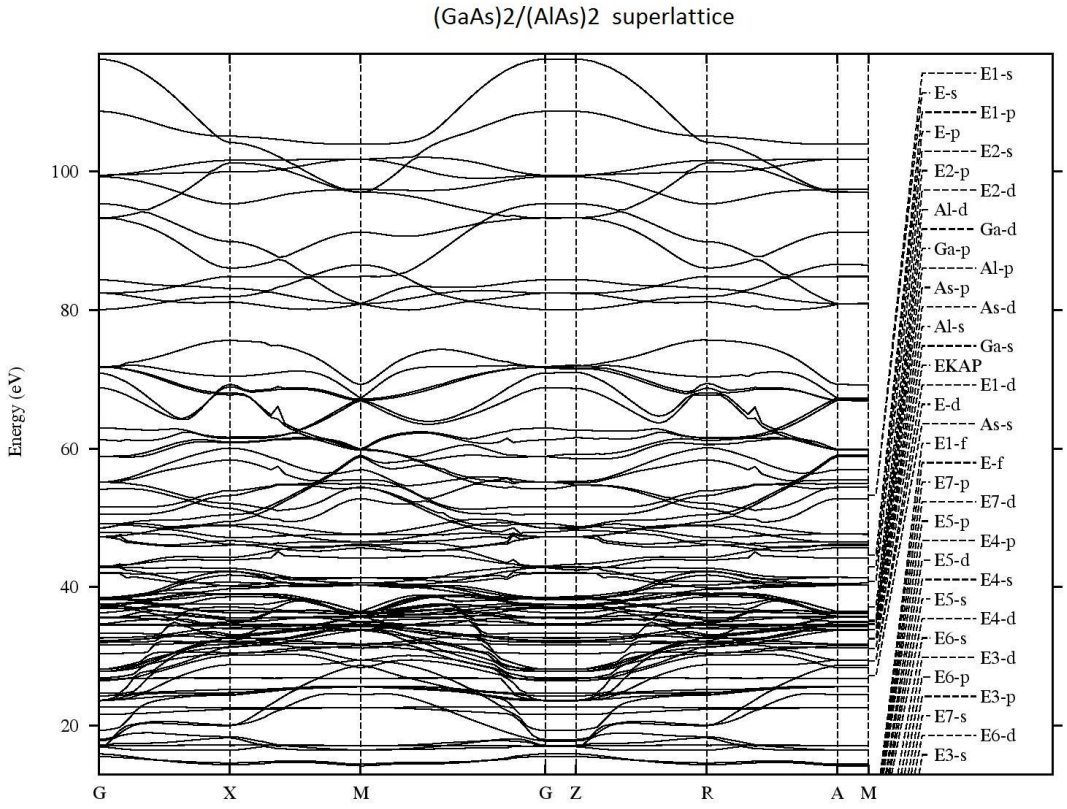


$(Gaas)_2/(AlAs)_2$ superlattice:

The period of this superlattice is nearly four times the lattice constant of its single crystals. In one period, there is two unit cells of gallium arsenide and two unit cells of aluminium arsenide. The growth axis of the superlattice is 001.

The band structure and density of states were plotted for it by using TB-LMTO code. The bands are very dense up to 40 ev. It is clear that the population of bands have further increased than the previous superlattice and band gaps have been narrower.

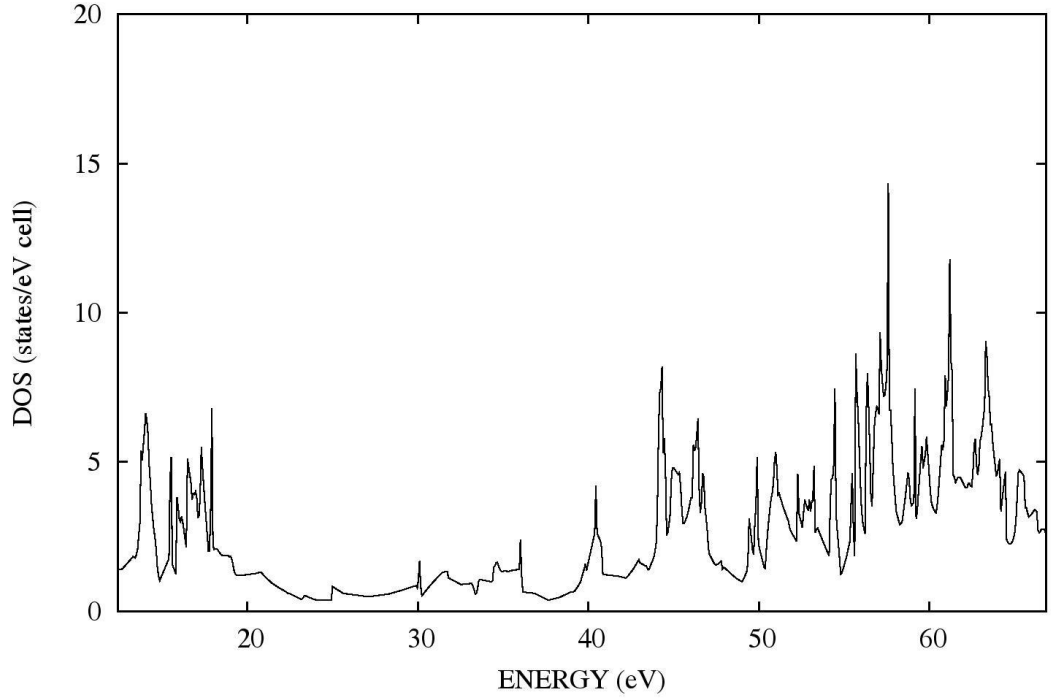
The density of states ranges up to 65ev. i.e. there are more number of states at higher energy compared to previous one. The density of states is lower from 20 to 40 ev. So, the electrons contribute less to transport properties in this energy range.



(GaAs)2/(AlAs)2 superlattice

/

F

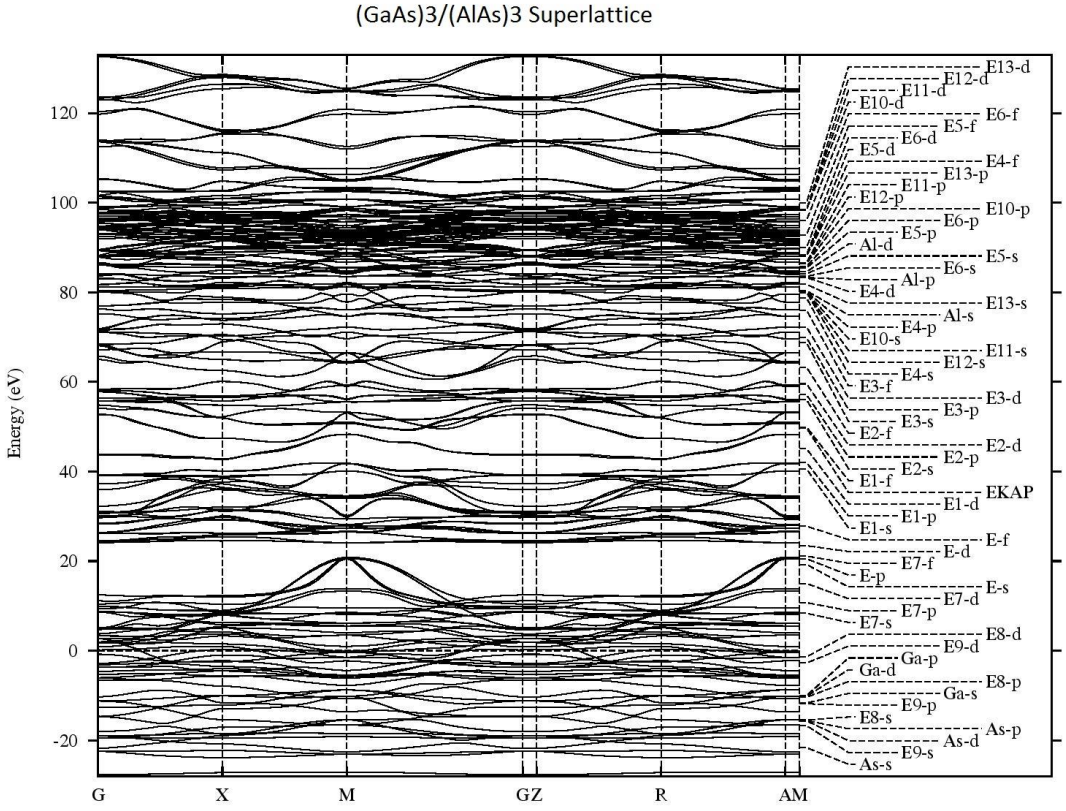


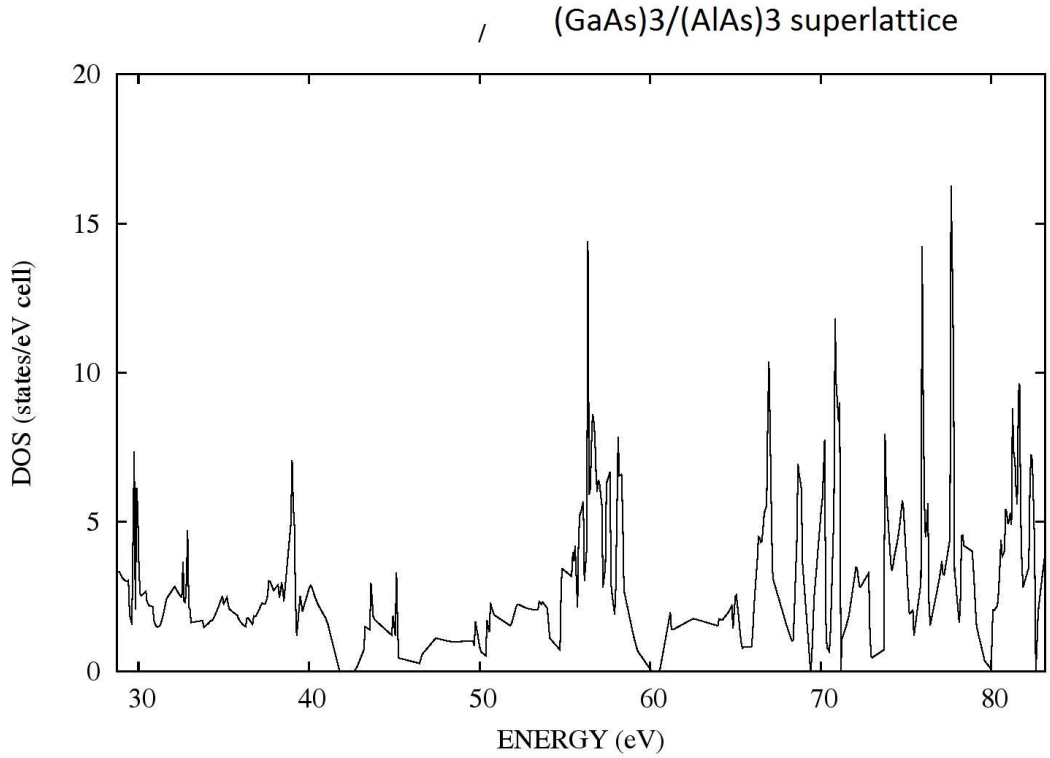
$(GaAs)_3/(AlAs)_3$:

Its periodicity is nearly six times of lattice constant of its single crystals. It consists of three unit cells of gallium arsenide and three unit cells of aluminium arsenide.

The band structures and density of states were plotted using TB-LMTO code. The plot shows that more sub bands have been formed than previous two superlattices and band gaps became narrower.

The density of states lies up to energy 85ev. This is due more number of bands are present in this case than previous superlattice.





So, it is concluded that increasing the periodicity in the superlattice in the growth direction, more sub bands are formed and bad gaps become narrow than that of single crystals. So, electronic properties are substantially changed.

Applications:

- The band gaps in superlattices can be changed according to our convenience by changing the periodicity of superlattice and thickness of the layers.
- Due to narrow band gap in superlattices, the intrasubbands transitions occur in far-infrared region which can be used in quantum cascade lasers.
- They show a differential electrical conductivity in the presence of electric fields. This occurs due to the shift of energy levels in the potential wells of the superlattice.
- Due to their extended periodicity, their Bloch oscillations can be observed. Since, the time period of Bloch oscillation will be less than scattering time. As the Bloch frequency is high in superlattices, they can be used as Tetra hertz generators.
- Narrow band gaps has also applications in electron spin polarizations.

Conclusion:

Electronic properties of semiconductors were studied through band structures generated by pseudo potential method using form factors found in literature. Also, using TB-LMTO code, the electronic properties of III-V semiconductors and its superlattices were studied by detail. It was found that these properties of superlattices significantly changes compared to its single crystals by extending the periodicity along growth direction.

References:

1. E. Fermi, Nuovo Cimento 11, 157 (1934)
2. H. J. Hellman, J. Chem. Phys. 3, 61 (1935)
3. Computational electronics, empirical pseudo potential method, Dragica Vasileska, associate professor , Arizona state university
4. D. Brust, Phys. Rev. B 4, 3497 (1971).
5. J. C. Phillips and L. Kleinman, Phys. Rev. 116, 287 (1959).
6. L. R. Saravia and D. Brust, Phys. Rev. 176, 915 (1968)
7. Electronic structure of hetero-crystalline superlattices, Nicola Manini, Giovanni Onida, Gabriele Faraone
8. L. Esaki and R. Tsu, IBM J. Res. Devel., 14, 61, 1970.
9. D. Mukherji and B. R. Niag, Phys. Rev. B, 12, 4438, 1975.
10. Ludeke, J. Vac. Sci. Technol., 10, 11, 1973.
11. D. Mukherji and B. R. Niag, Phys. Rev. B, 12, 4438, 1975.
12. R. Dingle, W. Wiegmann, and C. H. Henry, Phys. Rev. Lett., 33, 827, 1974.
13. M. Cardona and Peter Y. Yu, Fundamentals of Semiconductors, Fourth Edition, Springer.
14. F. Bloch, Z. Phys., 52, 555, 1929.
15. Richard J. Gonsalves, (2011) Computational Physics I,
16. J.C. Phillips, "Energy-Band Interpolation Scheme Based on a Pseudopotential," Phys. Rev. **112**, 685 (1958).
17. J.C. Phillips and L. Kleinman, "New Method for Calculating Wave Functions in Crystals and Molecules," Phys. Rev. **116**, 287 (1959).
18. L. Kleinman and J.C. Phillips, "Crystal Potential and Energy Bands of Semiconductors. III. Self-Consistent Calculations for Silicon," Phys. Rev. **118**, 1153 (1960).
19. Marvin L. Cohen and T.K. Bergstresser, "Band Structures and Pseudopotential Form Factors for Fourteen Semiconductors of the Diamond and Zinc-blende Structures," Phys. Rev. **141**, p. 789 (1966)